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NEWS 7 DEC 21 IPC search and display fields enhanced in CA/CAplus with the  
IPC reform  
NEWS 8 DEC 23 New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/  
USPAT2  
NEWS 9 JAN 13 IPC 8 searching in IFIPAT, IFIUDB, and IFICDB  
NEWS 10 JAN 13 New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to  
INPADOC  
NEWS 11 JAN 17 Pre-1988 INPI data added to MARPAT  
NEWS 12 JAN 17 IPC 8 in the WPI family of databases including WPIFV  
NEWS 13 JAN 30 Saved answer limit increased  
NEWS 14 JAN 31 Monthly current-awareness alert (SDI) frequency  
added to TULSA

NEWS EXPRESS JANUARY 03 CURRENT VERSION FOR WINDOWS IS V8.01,  
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AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.  
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SINCE FILE TOTAL  
ENTRY SESSION

FULL ESTIMATED COST

0.21

0.21

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STRUCTURE FILE UPDATES: 6 FEB 2006 HIGHEST RN 873652-66-5  
DICTIONARY FILE UPDATES: 6 FEB 2006 HIGHEST RN 873652-66-5

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\*\*\*\*\*  
\*  
\* The CA roles and document type information have been removed from \*  
\* the IDE default display format and the ED field has been added, \*  
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\* available and contains the CA role and document type information. \*  
\*  
\*\*\*\*\*

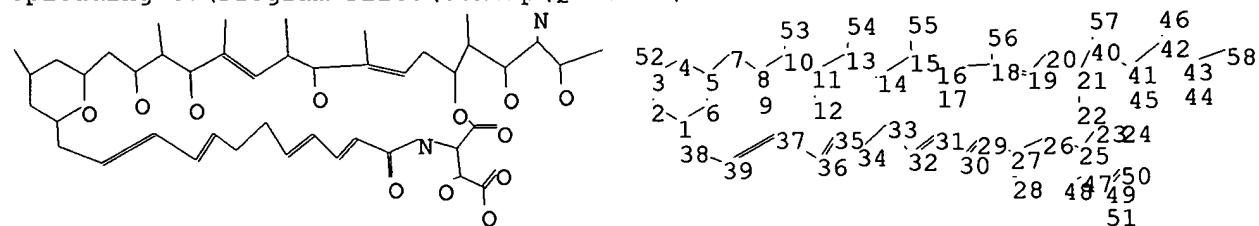
Structure search iteration limits have been increased. See HELP SLIMITS  
for details.

REGISTRY includes numerically searchable data for experimental and  
predicted properties as well as tags indicating availability of  
experimental property data in the original document. For information  
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10521930b.str



chain nodes :

9 12 17 24 28 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55

56 57 58

ring nodes :

1 2 3 4 5 6 7 8 10 11 13 14 15 16 18 19 20 21 22 23 25 26 27  
29 30 31 32 33 34 35 36 37 38 39

chain bonds :

3-52 8-9 10-53 11-12 13-54 15-55 16-17 18-56 21-40 23-24 25-47 27-28  
40-41 40-57 41-42 41-45 42-43 42-46 43-44 43-58 47-48 47-49 49-50 49-51

ring bonds :

1-2 1-6 1-38 2-3 3-4 4-5 5-6 5-7 7-8 8-10 10-11 11-13 13-14 14-15  
15-16 16-18 18-19 19-20 20-21 21-22 22-23 23-25 25-26 26-27 27-29 29-30  
30-31 31-32 32-33 33-34 34-35 35-36 36-37 37-39 38-39

exact/norm bonds :

1-2 1-6 1-38 2-3 3-4 4-5 5-6 5-7 7-8 8-9 8-10 10-11 11-12 11-13 13-14  
14-15 15-16 16-17 16-18 18-19 19-20 20-21 21-22 22-23 23-24 23-25 25-26  
26-27 27-28 27-29 29-30 30-31 31-32 32-33 33-34 34-35 35-36 36-37 37-39  
38-39 41-45 42-46 43-44 47-48 49-50 49-51

exact bonds :

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47-49

Match level :

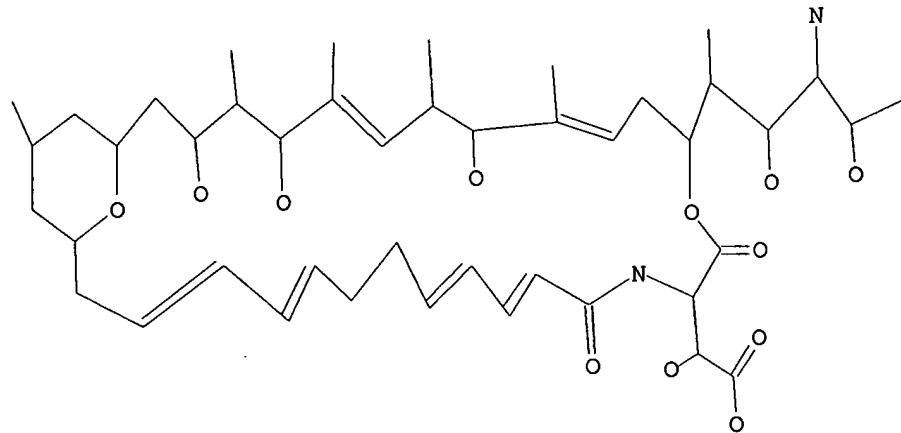
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 10:Atom  
11:Atom 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom 19:Atom  
20:Atom 21:Atom 22:Atom 23:Atom 24:CLASS 25:Atom 26:Atom 27:Atom 28:CLASS  
29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom  
38:Atom 39:Atom 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS 45:CLASS  
46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS 53:CLASS  
54:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 13:14:02 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 0 TO 0

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s 11 full  
FULL SEARCH INITIATED 13:14:07 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 13 TO ITERATE

100.0% PROCESSED 13 ITERATIONS 4 ANSWERS  
SEARCH TIME: 00.00.01

L3 4 SEA SSS FUL L1

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
FULL ESTIMATED COST ENTRY SESSION  
166.94 167.15

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=> s 13 full  
L4 3 L3

=> d ibib abs hitstr 1-3

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 2004:80497 CAPLUS  
DOCUMENT NUMBER: 140:139542  
TITLE: Chondropsin-class antitumor vacuolar ATPase inhibitor compounds, compositions, and methods of use  
INVENTOR(S): Boyd, Michael R.; Gustafson, Kirk R.  
PATENT ASSIGNEE(S): The Government of the United States of America, Represented by the Secretary Dept. of Health and Human Services, USA  
SOURCE: PCT Int. Appl., 54 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004009079	A1	20040129	WO 2003-US23290	20030724
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2493821	AA	20040129	CA 2003-2493821	20030724
EP 1542674	A1	20050622	EP 2003-751813	20030724
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005176810	A1	20050811	US 2003-521930	20030724
PRIORITY APPLN. INFO.:			US 2002-398092P	P 20020724
			WO 2003-US23290	W 20030724

OTHER SOURCE(S): MARPAT 140:139542

AB The invention discloses the title compds., compns. comprising a therapeutically effective amount of at least one of them, alone or in combination with at least one addnl. therapeutic agent, and methods of preventing or treating cancer and a condition treatable by the inhibition of vacuolar-type (H<sup>+</sup>)-ATPase. Isolation and purification of poecillastrin A is described.

IT **471913-55-0P**, Poecillastrin A

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses) (chondropsin-class antitumor vacuolar ATPase inhibitor compds., compns., and methods of use)

RN 471913-55-0 CAPLUS

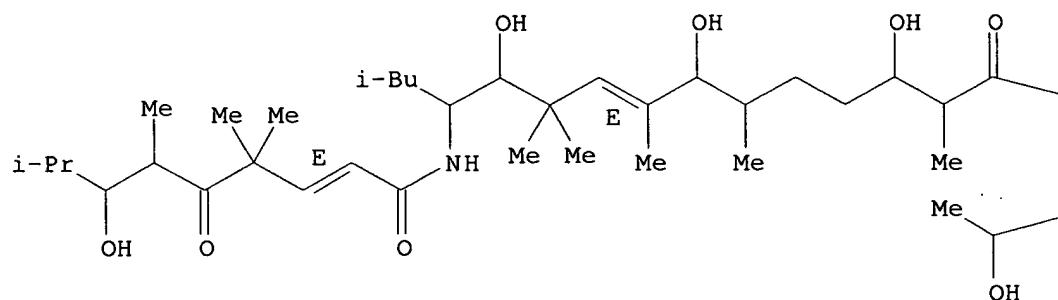
CN 14,34-Dioxa-17-azabicyclo[28.3.1]tetratriaconta-6,10,19,21,25,27-hexaene-16-acetic acid, 13-[2,4-dihydroxy-1-methyl-3-[(8E)-3,7,11-trihydroxy-12-[(2E)-7-hydroxy-4,4,6,8-tetramethyl-1,5-dioxo-2-nonenyl]amino]-2,6,8,10,10,14-hexamethyl-1-oxo-8-pentadecenyl]amino]pentyl]- $\alpha$ ,3,5,9-tetrahydroxy-29-methoxy-4,6,8,10,32-pentamethyl-15,18-dioxo-, (6E,10E,19E,21E,25E,27E)-(-) (9CI) (CA INDEX NAME)

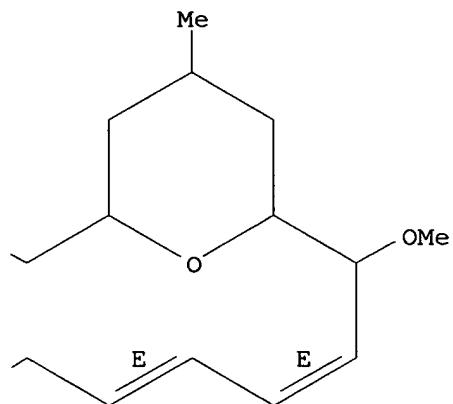
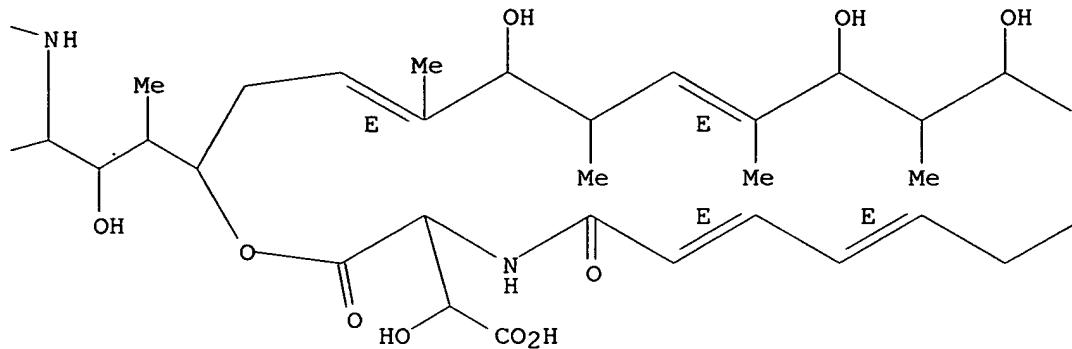
Rotation (-).

Double bond geometry as described by E or Z.

Currently available stereo shown.

PAGE 1-A





IT 651726-41-9 651726-42-0 651726-43-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

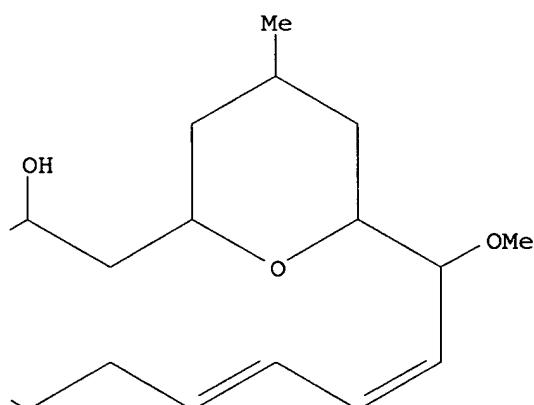
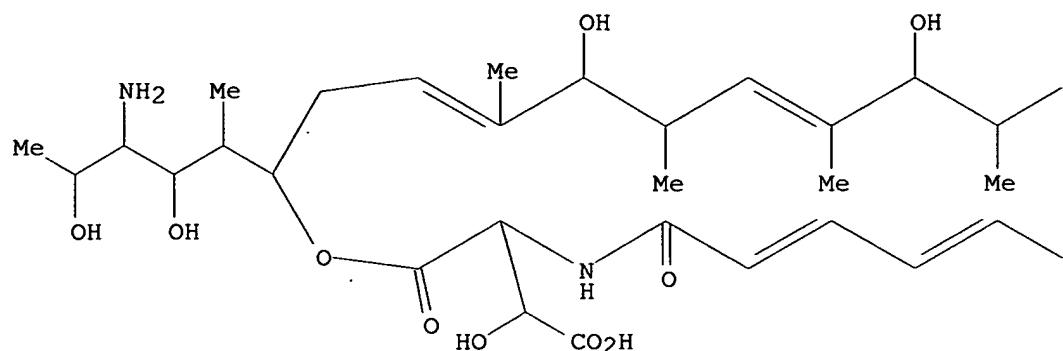
(chondropsin-class antitumor vacuolar ATPase inhibitor compds., compns., and methods of use)

RN 651726-41-9 CAPLUS

CN 14,34-Dioxa-17-azabicyclo[28.3.1]tetratriaconta-6,10,19,21,25,27-hexaene-16-acetic acid, 13-(3-amino-2,4-dihydroxy-1-methylpentyl)- $\alpha$ ,3,5,9-tetrahydroxy-29-methoxy-4,6,8,10,32-pentamethyl-15,18-dioxo- (9CI) (CA INDEX NAME)

Double bond geometry unknown.

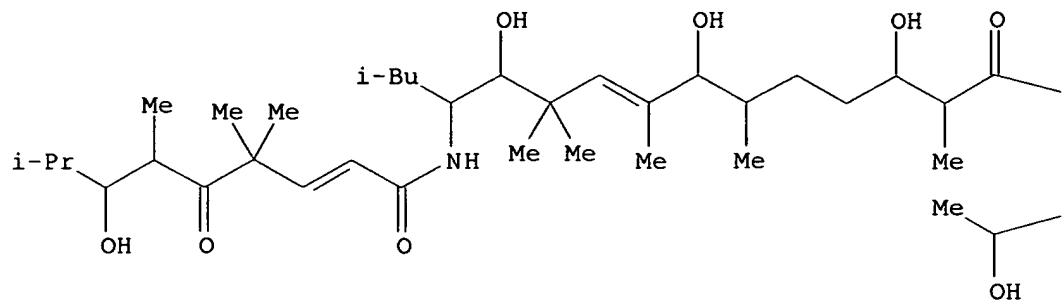
Currently available stereo shown.



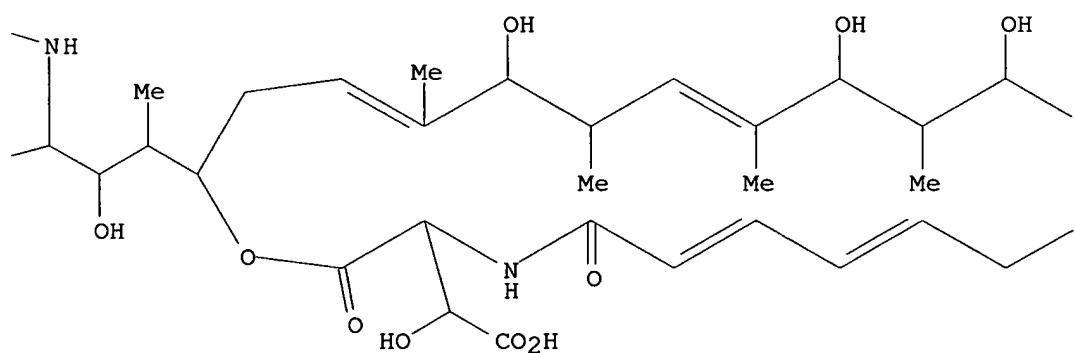
RN 651726-42-0 CAPLUS  
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Double bond geometry unknown.  
 Currently available stereo shown.

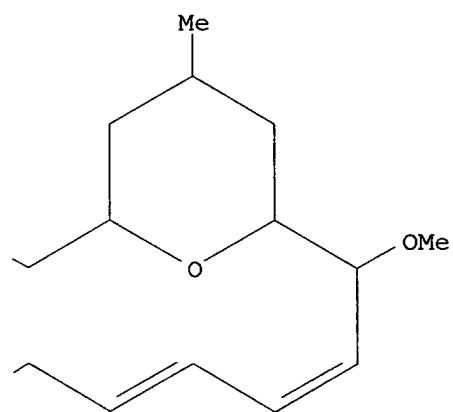
PAGE 1-A



PAGE 1-B



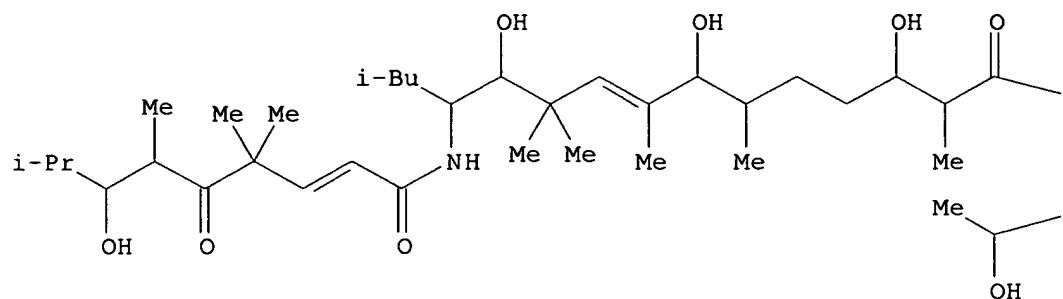
PAGE 1-C



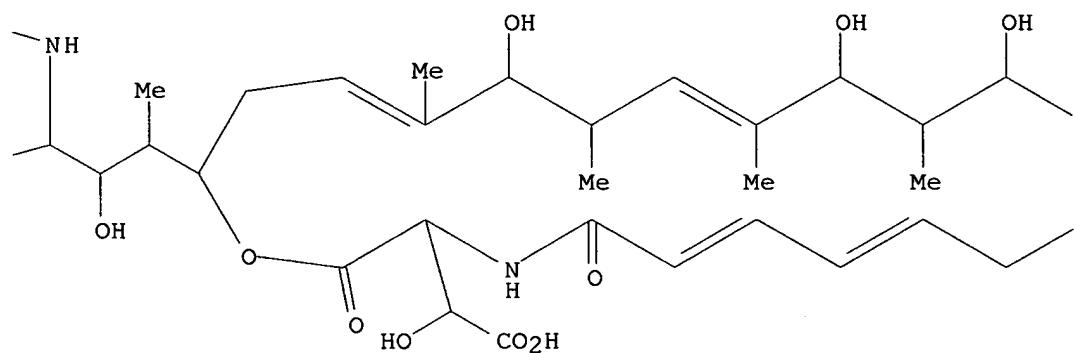
RN 651726-43-1 CAPLUS  
CN 14,34-Dioxa-17-azabicyclo[28.3.1]tetratriaconta-6,10,19,21,25,27-hexaene-16-acetic acid, 13-[2,4-dihydroxy-1-methyl-3-[[3,7,11-trihydroxy-12-[[7-hydroxy-4,4,6,8-tetramethyl-1,5-dioxo-2-nonenyl]amino]-2,6,8,10,10,14-hexamethyl-1-oxo-8-pentadecenyl]amino]pentyl]- $\alpha$ ,3,5,9-tetrahydroxy-29-methoxy-4,6,8,10,32-pentamethyl-15,18-dioxo-, (1S,30S,32S)- (9CI) (CA INDEX NAME)

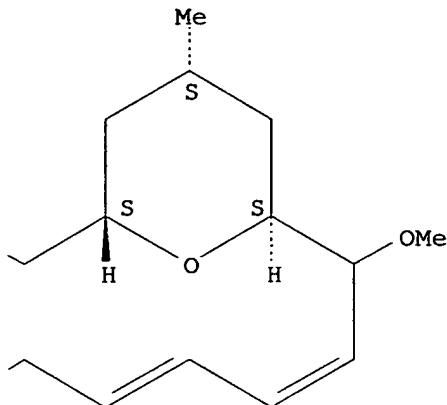
Absolute stereochemistry.  
Double bond geometry unknown.  
Currently available stereo shown.

PAGE 1-A



PAGE 1-B





REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2003:871548 CAPLUS  
 DOCUMENT NUMBER: 140:87244  
 TITLE: Identification of a New Chondropsin Class of Antitumor Compound That Selectively Inhibits V-ATPases  
 Bowman, Emma Jean; Gustafson, Kirk R.; Bowman, Barry J.; Boyd, Michael R.  
 AUTHOR(S):  
 CORPORATE SOURCE: Department of Molecular, Cell and Developmental Biology, University of California, Santa Cruz, CA, 95064, USA  
 SOURCE: Journal of Biological Chemistry (2003), 278(45), 44147-44152  
 CODEN: JBCHA3; ISSN: 0021-9258  
 PUBLISHER: American Society for Biochemistry and Molecular Biology  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The authors identify a new naturally occurring class of inhibitor of vacuolar H<sup>+</sup>-ATPases (V-ATPases) isolated from vacuolar membranes of *Neurospora crassa* and from chromaffin granule membranes of *Bos taurus*. To date, the new class includes six chondropsins and poecillastrin A, large polyketide-derived macrolide lactams with 33-37 membered rings. In the National Cancer Institute's 60-cell screen the chondropsin class showed a tumor cell growth inhibitory fingerprint essentially indistinguishable from that of the baflomycin/concanamycin and the salicylihalamide/lobatamide classes of well-established V-ATPase inhibitors. Half-maximal inhibition of V-ATPase activity in vitro occurred at 0.04-0.7 μM for the fungal vacuolar V-ATPase and at 0.4 to >10 μM for the chromaffin granule V-ATPase. Thus, the new inhibitors are somewhat less potent than the other two classes, which typically have Ki values of <10 nM for V-ATPases, and the new inhibitors differ from the other two classes in their specificity. The baflomycin class inhibits all eucaryotic V-ATPases, the salicylihalamide class inhibits mammalian V-ATPases but not fungal V-ATPases, and the new chondropsin class inhibits the *N. crassa* V-ATPase better than the chromaffin granule V-ATPase. Two mutations in the *N. crassa* V-ATPase that affect the binding of baflomycin had small but reproducible effects on the affinity of chondropsins for the V-ATPase, suggesting the possibility of a similar mechanism of inhibition.

IT 471913-55-0, Poecillastrin A  
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(identification of a new chondropsin class of antitumor compound that selectively inhibits V-ATPases)

RN 471913-55-0 CAPLUS

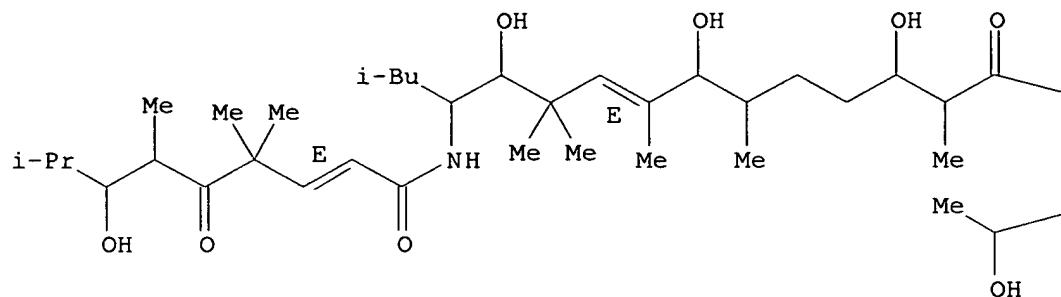
CN 14,34-Dioxa-17-azabicyclo[28.3.1]tetratriaconta-6,10,19,21,25,27-hexaene-16-acetic acid, 13-[2,4-dihydroxy-1-methyl-3-[(8E)-3,7,11-trihydroxy-12-[(2E)-7-hydroxy-4,4,6,8-tetramethyl-1,5-dioxo-2-nonenyl]amino]-2,6,8,10,10,14-hexamethyl-1-oxo-8-pentadecenyl]amino]pentyl]- $\alpha$ ,3,5,9-tetrahydroxy-29-methoxy-4,6,8,10,32-pentamethyl-15,18-dioxo-, (6E,10E,19E,21E,25E,27E)-(-) - (9CI) (CA INDEX NAME)

Rotation (-).

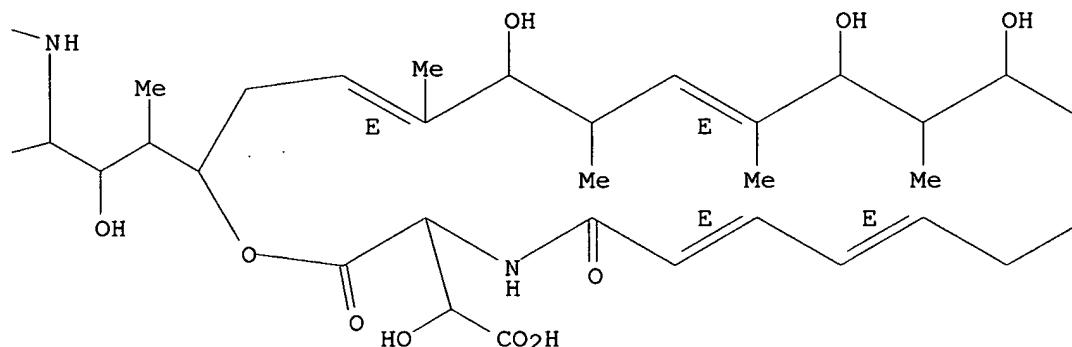
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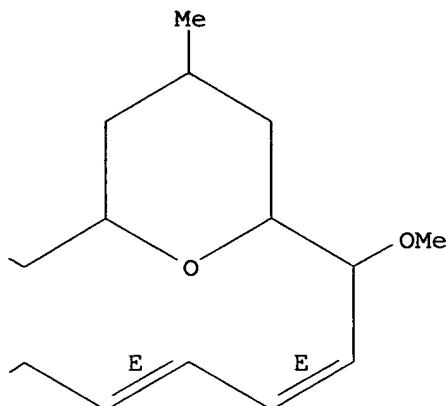
Currently available stereo shown.

PAGE 1-A



PAGE 1-B





REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:635740 CAPLUS

DOCUMENT NUMBER: 137:310745

TITLE: Application of High-Field NMR and Cryogenic Probe Technologies in the Structural Elucidation of Poecillastrin A, a New Antitumor Macrolide Lactam from the Sponge Poecillastra Species

AUTHOR(S): Rashid, Mohammad A.; Gustafson, Kirk R.; Crouch, Ronald C.; Graweiss, Amiram; Pannell, Lewis K.; Van, Que N.; Boyd, Michael R.

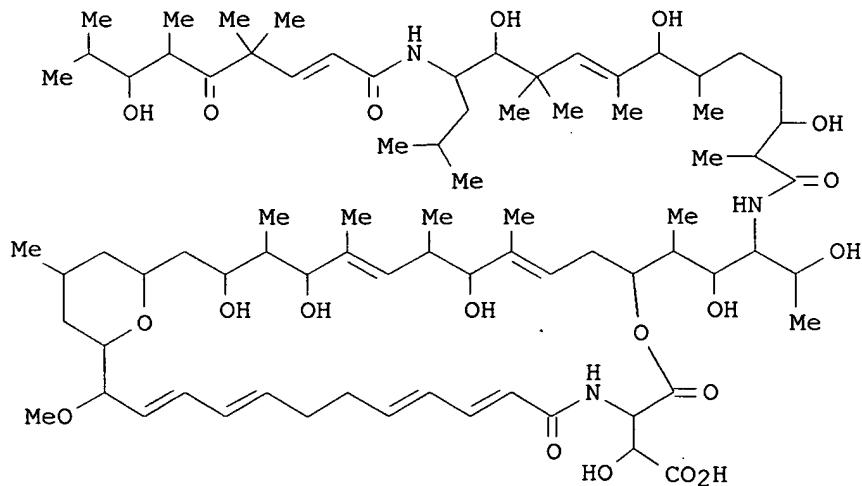
CORPORATE SOURCE: Molecular Targets Drug Discovery Program, Center for Cancer Research, National Cancer Institute, Frederick, MD, 21702-1201, USA

SOURCE: Organic Letters (2002), 4(19), 3293-3296  
CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal  
LANGUAGE: English

GI



AB Poecillastrin A (I), a new polyketide-derived macrolide lactam, was isolated from a deep-water collection of the marine sponge Poecillastra species. The structure of I was assigned using NMR data acquired at 500 MHz with an inverse-detection cryogenic probe and at 800 MHz with a room-temperature probe.

IT **471913-55-0P, Poecillastrin A**

RL: NPO (Natural product occurrence); PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PUR (Purification or recovery); PYP (Physical process); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process)  
(high-field NMR and cryogenic probe technologies in the structural elucidation of poecillastrin A from Poecillastra species)

RN 471913-55-0 CAPLUS

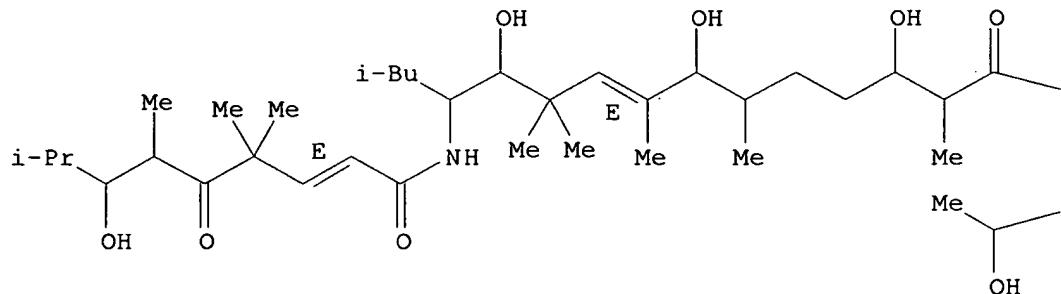
CN 14,34-Dioxa-17-azabicyclo[28.3.1]tetratriaconta-6,10,19,21,25,27-hexaene-16-acetic acid, 13-[2,4-dihydroxy-1-methyl-3-[(8E)-3,7,11-trihydroxy-12-[(2E)-7-hydroxy-4,4,6,8-tetramethyl-1,5-dioxo-2-nonenyl]amino]-2,6,8,10,10,14-hexamethyl-1-oxo-8-pentadecenyl]amino]pentyl]- $\alpha$ ,3,5,9-tetrahydroxy-29-methoxy-4,6,8,10,32-pentamethyl-15,18-dioxo-, (6E,10E,19E,21E,25E,27E)-(-) - (9CI) (CA INDEX NAME)

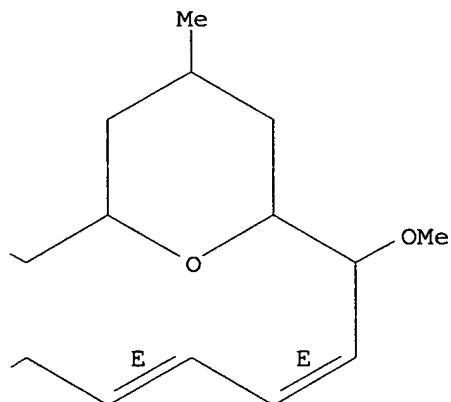
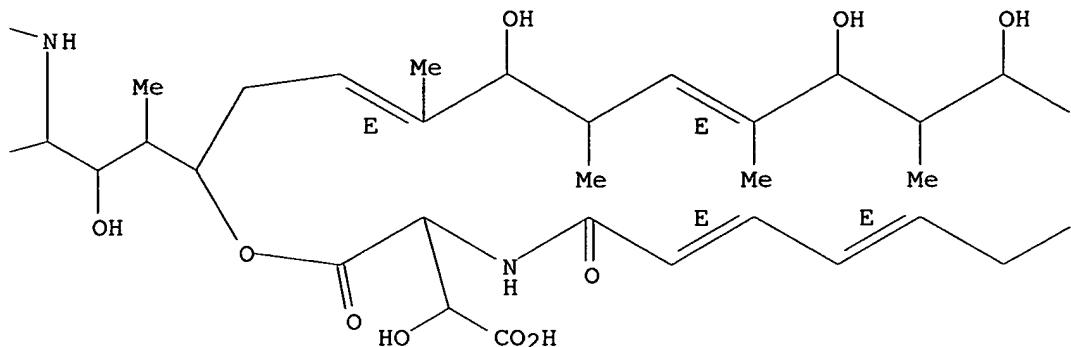
Rotation (-).

Double bond geometry as described by E or Z.

Currently available stereo shown.

PAGE 1-A





**REFERENCE COUNT:**

21

THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file marpat

COST IN U.S. DOLLARS

SINCE FILE TOTAL  
ENTRY SESSION

**FULL ESTIMATED COST**

16.71 183.86

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL  
ENTRY SESSION

CA SUBSCRIBER PRICE

-2.25 -2.25

FILE 'MARPAT' ENTERED AT 13:16:06 ON 07 FEB 2006  
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FILE CONTENT: 1969-PRESENT (VOL 144 ISS 6 (20060205/ED)

SOME MARPAT RECORDS ARE DERIVED FROM INPI DATA FOR 1969-1987

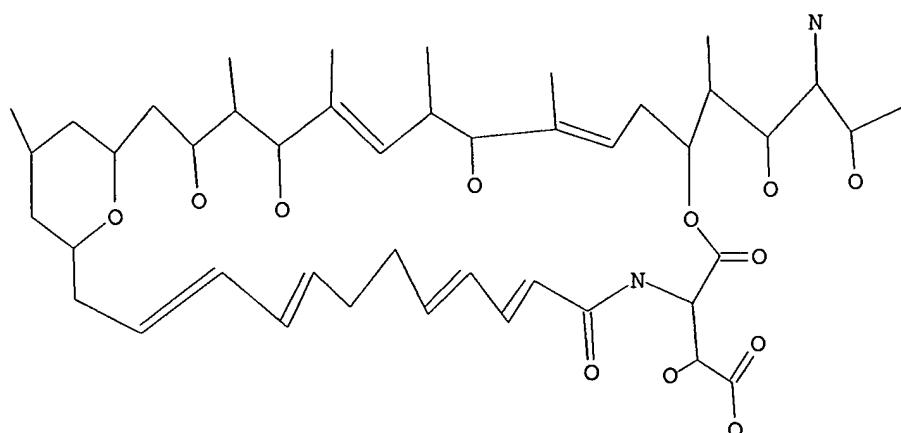
MOST RECENT CITATIONS FOR PATENTS FROM FIVE MAJOR ISSUING AGENCIES  
(COVERAGE TO THESE DATES IS NOT COMPLETE):

US 6965040 15 NOV 2005  
DE 1020040544 17 NOV 2005  
EP 1600439 30 NOV 2005  
JP 2005336157 08 DEC 2005  
WO 2005121067 22 DEC 2005

Expanded G-group definition display now available.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

=> d 11  
L1 HAS NO ANSWERS  
L1 STR



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=> s 11 full  
FULL SEARCH INITIATED 13:16:35 FILE 'MARPAT'  
FULL SCREEN SEARCH COMPLETED - 189 TO ITERATE

100.0% PROCESSED 189 ITERATIONS 1 ANSWERS  
SEARCH TIME: 00.00.01

L5 1 SEA SSS FUL L1

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L5 ANSWER 1 OF 1 MARPAT COPYRIGHT 2006 ACS on STN  
ACCESSION NUMBER: 140:139542 MARPAT  
TITLE: Chondropsin-class antitumor vacuolar ATPase inhibitor  
compounds, compositions, and methods of use  
INVENTOR(S): Boyd, Michael R.; Gustafson, Kirk R.  
PATENT ASSIGNEE(S): The Government of the United States of America,  
Represented by the Secretary Dept. of Health and Human  
Services, USA  
SOURCE: PCT Int. Appl., 54 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English

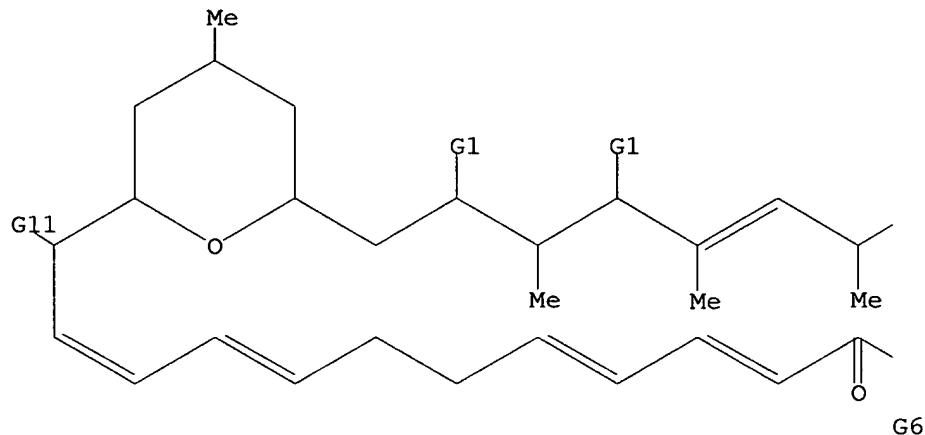
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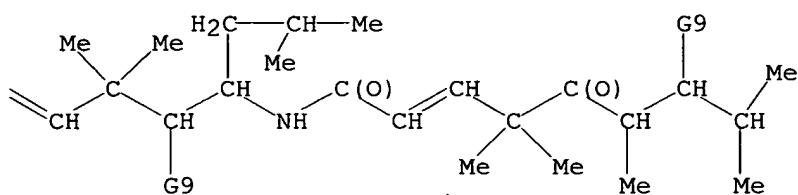
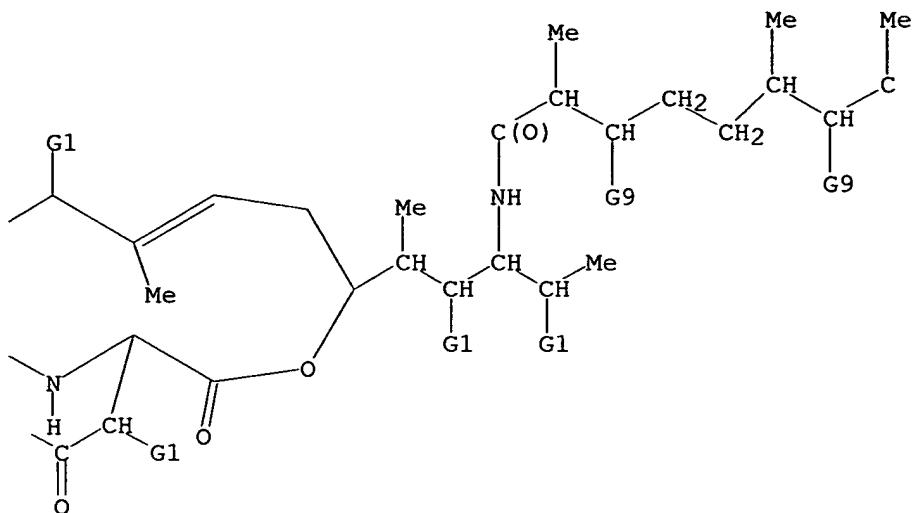
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009079	A1	20040129	WO 2003-US23290	20030724
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2493821	AA	20040129	CA 2003-2493821	20030724
EP 1542674	A1	20050622	EP 2003-751813	20030724
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK			
US 2005176810	A1	20050811	US 2003-521930	20030724
PRIORITY APPLN. INFO.:				
			US 2002-398092P	20020724
			WO 2003-US23290	20030724

AB The invention discloses the title compds., compns. comprising a therapeutically effective amount of at least one of them, alone or in combination with at least one addnl. therapeutic agent, and methods of preventing or treating cancer and a condition treatable by the inhibition of vacuolar-type (H<sup>+</sup>)-ATPase. Isolation and purification of poecillastrin A is described.

**MSTR 1**





G1 = OH

G6 = OH

Patent location:

claim 1

Note: or pharmaceutically acceptable salts or prodrugs

**REFERENCE COUNT:**

3

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

$$\Rightarrow \log y$$

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DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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